WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Wednesday, December 12, 2007

Hide?	Set Name	Query	Hit Count
		DB=PGPB,USPT; PLUR=YES; OP=ADJ	
☐	L4	(pyrrolo adj3 pyridazine)	8
☐	L3	L2 and (pyrrolo adj3 pyridazine)	0
☐	L2	514/525.06.icls. or 514/252.06.ccls. or 544/236.icls. or 544/236.ccls.	910
☐	L1	6342601.pn.	1

END OF SEARCH HISTORY

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     FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007
L1                STRUCTURE UPLOADED
L2              0 S L1
L3            237 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007
L4              7 S L3

     FILE 'REGISTRY' ENTERED AT 10:28:45 ON 12 DEC 2007
L5                STRUCTURE UPLOADED
L6              1 S L5
L7             86 S L5 SSS FULL

     FILE 'CAPLUS' ENTERED AT 10:29:37 ON 12 DEC 2007
L8             19 S L7
L9             18 S L8 NOT L4

     FILE 'REGISTRY' ENTERED AT 11:33:03 ON 12 DEC 2007
L10               STRUCTURE UPLOADED
L11             3 S L10
L12            54 S L10 SSS FULL

     FILE 'CAPLUS' ENTERED AT 11:36:06 ON 12 DEC 2007
L13             4 S L12
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=> file registry
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY     SESSION
FULL ESTIMATED COST                                         0.21        0.21

FILE 'REGISTRY' ENTERED AT 10:19:12 ON 12 DEC 2007
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provided by InfoChem.

STRUCTURE FILE UPDATES:   11 DEC 2007  HIGHEST RN 957570-32-0
DICTIONARY FILE UPDATES:  11 DEC 2007  HIGHEST RN 957570-32-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10520962broad.str
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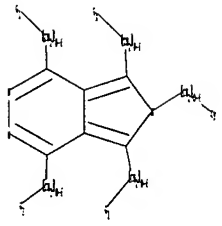

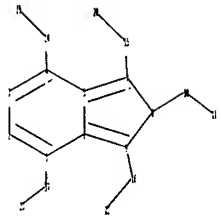

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10 11 14 15 16 17 19 20 22 23
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-17 4-14 7-15 8-10 9-16 10-11 14-19 15-20 16-22 17-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 14-19 15-20 16-22 17-23

exact bonds :
1-17 4-14 7-15 8-10 9-16

G1:H,Cy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 22:CLASS
23:CLASS

L1 STRUCTURE UPLOADED

=> s l1
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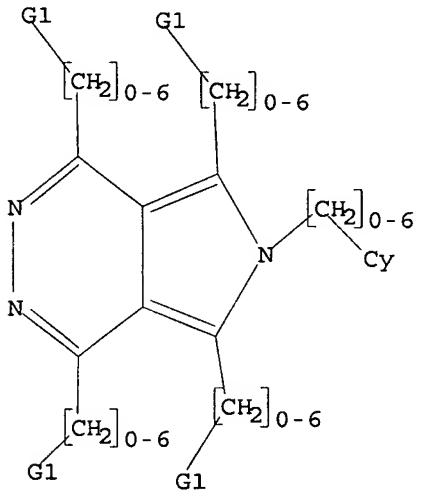
SAMPLE SCREEN SEARCH COMPLETED - 78197 TO ITERATE

2.6% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 1547303 TO 1580577
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Cy

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 10:19:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1557677 TO ITERATE

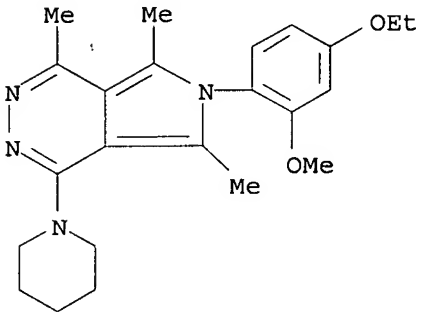
64.2% PROCESSED 1000000 ITERATIONS 237 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.16

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 1557677 TO 1557677
PROJECTED ANSWERS: 312 TO 426

L3 237 SEA SSS FUL L1

=> d l3 scan

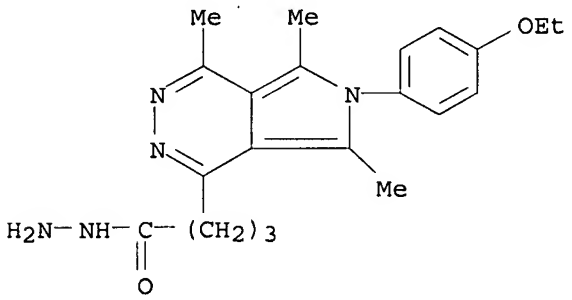
L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxy-2-methoxyphenyl)-1,5,7-trimethyl-4-(1-piperidinyl)-
MF C23 H30 N4 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

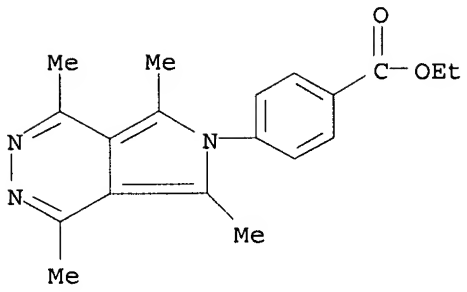
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine-1-butanoic acid, 6-(4-ethoxyphenyl)-4,5,7-trimethyl-, hydrazide
MF C21 H27 N5 O2



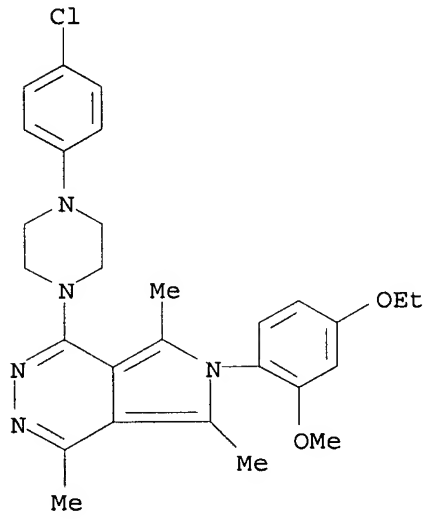
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 4-(1,4,5,7-tetramethyl-6H-pyrrolo[3,4-d]pyridazin-6-yl)-, ethyl ester
MF C19 H21 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 237 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 1-[4-(4-chlorophenyl)-1-piperazinyl]-6-(4-ethoxy-2-methoxyphenyl)-4,5,7-trimethyl-
MF C28 H32 Cl N5 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.45	173.66

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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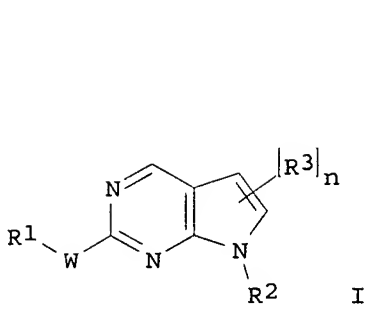
FILE COVERS 1907 - 12 Dec 2007 VOL 147 ISS 25
FILE LAST UPDATED: 11 Dec 2007 (20071211/ED)

=> s l3
L4 7 L3

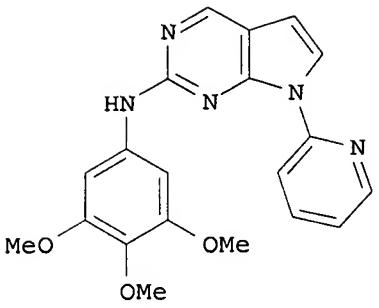
=> d l4 1-7 ti abs bib

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
TI Expedited SAR study of high-affinity ligands to the α2δ subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology
AB The SAR of the lead compound 3, a novel ligand for the α2δ subunit of voltage-gated calcium channels, was rapidly explored. Utilizing a parallel solution-phase Sn2Ar coupling approach, a focused library was obtained. The library was evaluated in vitro and afforded a series of analogs with improved potencies. The SAR trends of the library are also described.
AN 2005:1342000 CAPLUS <<LOGINID::20071212>>
DN 144:100381
TI Expedited SAR study of high-affinity ligands to the α2δ subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology
AU Chen, Chixu; Stearns, Brian; Hu, Tao; Anker, Naomi; Santini, Angelina; Arruda, Jeannie M.; Campbell, Brian T.; Datta, Purabi; Aiyar, Jayashree; Munoz, Benitio
CS Department of Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(3), 746-749
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:100381
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
TI Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation
GI



I



II

AB The invention provides compds. I [n = 0-2; W = NR4, S, O, SO, SO2 (wherein R4 = H, alkyl); R1 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R2 = arylalkyl, heteroarylalkyl, cycloalkylalkyl, etc.; R3 = halo, OH, XSR5, etc. (X = a bond, alkylene; R5 = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to induce undifferentiated keratinocytes to differentiate into terminally differentiated keratinocytes. The invention further provides compds. for the treatment of diseases or disorders associated with casein kinase II (CK2), TANK-binding kinase 1 (TBK1) and NIMA-related kinase 9 (NEK9). Over 200 compds. I were prepared E.g., a 4-step synthesis of II, starting from 5-bromo-2,4-dichloropyrimidine, was given.

AN 2005:1220346 CAPLUS <<LOGINID::20071212>>

DN 143:477978

TI Preparation of substituted pyrrolo[2,3-d]pyrimidines as inducers of keratinocyte differentiation

IN Hong, Jiyong; Gray, Nathanael S.; Schultz, Peter

PA IRM LLC, Bermuda

SO PCT Int. Appl., 53 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005107760	A1	20051117	WO 2005-US15118	20050429

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2004-567346P P 20040430

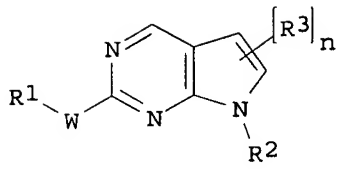
OS CASREACT 143:477978; MARPAT 143:477978

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

TI Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors

GI



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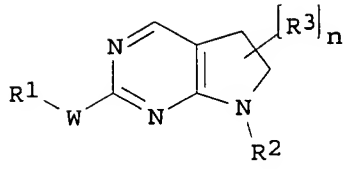

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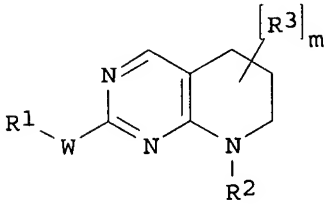

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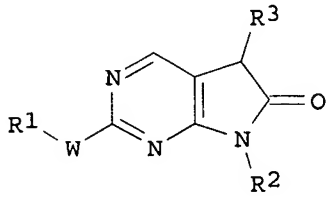

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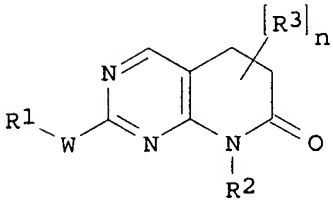


V

AB The invention provides a novel class of compds. I-V [n = 0-2; m = 0-3; W = NR4, S, O, SO, SO2 (wherein R4 = H, alkyl); R1 = (un)substituted (hetero)arylakyl, (hetero)cycloalkyl; R2 = (un)substituted (hetero)arylakyl, (hetero)cycloalkyl; R3 = halo, OH, XSR5, etc. (X = a bond, alkylene; R5 = H, alkyl, cycloalkylalkyl)], pharmaceutical compns. comprising such compds. and methods of using such compds. to treat or prevent diseases or disorders associated with abnormal or deregulated kinase activity, particularly diseases or disorders that involve abnormal activation of the FAK, Abl, BCR-Abl, PDGF-R, c-Kit, NPM-ALK, Flt-3, JAK2 and c-Met kinases. Over 200 compds. I-V were prepared and characterized. The preparation of the compds. I is illustrated in examples. E.g., synthesis of I [R1 = 3,4,6-(MeO)3C6H2; R2 = 2-pyridyl; R3 = H; W = NH], starting from 5-bromo-2,4-dichloropyrimidine, was given. The compds. I-V were tested against various kinases. For example, they inhibit the enzyme activity by 50% (IC50), in a concentration of from 0.001 to 0.5 μM, especially from 0.01 to 0.1 μM.

AN 2005:962258 CAPLUS <<LOGINID::20071212>>
DN 143:266947

TI Preparation of pyrrolopyrimidines and their analogs as protein kinase inhibitors

IN Choi, Ha-Soon; Wang, Zhicheng; Gray, Nathanael Schiander; Gu, Xiang-Ju; He, Xiaohui; He, Yun; Jiang, Tao; Liu, Yi; Richmond, Wendy; Sim, Taebo; Yang, Kunyong
PA IRM LLC, Bermuda

SO PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

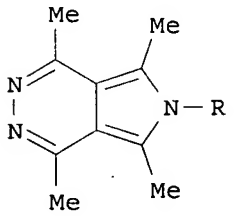
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005080393	A1	20050901	WO 2005-US4630	20050214

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005214352	A1	20050901	AU 2005-214352	20050214
CA 2553785	A1	20050901	CA 2005-2553785	20050214
EP 1713806	A1	20061025	EP 2005-713510	20050214
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
CN 1918158	A	20070221	CN 2005-80004895	20050214
BR 2005007668	A	20070717	BR 2005-7668	20050214
JP 2007522241	T	20070809	JP 2006-553321	20050214
MX 2006PA09158	A	20061110	MX 2006-PA9158	20060811
IN 2006CN02987	A	20070608	IN 2006-CN2987	20060814
US 2007225306	A1	20070927	US 2007-589099	20070611
PRAI US 2004-544944P	P	20040214		
WO 2005-US4630	W	20050214		

OS MARPAT 143:266947
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the α2δ subunit of voltage-gated calcium channels
GI



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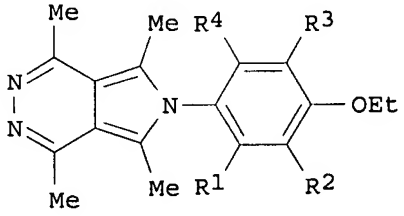
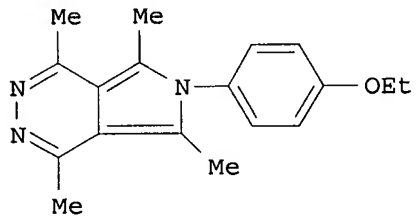


II

AB 2H-pyrrolo[3,4-c]pyridazines I (R = 4-EtOC6H4, 2-EtO-5-pyridinyl, 5-EtO-2-pyridinyl, 5-EtO-2-pyrazinyl, 4-EtO-1-pyridazinyl, 2-EtO-5-pyrimidinyl, etc.) such as II (R1 = H, MeO, Et, H2C:CH, Me, MeS, EtO, F; R2 = H, Me; R3 = H, Me, Cl, HOCH2; R4 = H, Me) are prepared as ligands for the α2δ subunit of voltage-gated calcium channels. Ortho-substituents capable of electron-donation increase the binding of II to the α2δ subunit of voltage-gated calcium channels; electron-withdrawing substituents in the ortho-position of II decrease binding significantly. II (R1 = MeO; R2 = R3 = R4 = H) binds to the α2δ subunit of voltage-gated calcium channels from A710 cells with an IC50 value of 4 nM. Testing of tritiated ligand II (R1 = TCH2TCH; R2 = R3 = R4 = H) in purified human α2δ voltage-gated calcium channel subunits indicates that II displace Gabapentin from the α2δ subunit of voltage-gated calcium channels, and thus act as Gabapentin mimics in vitro. In the preparation of II (R1 = Et; R2 = R3 = R4 = H), a novel metal-free hydrogenation is used using hydrazine as the reductant; the reduction is effective in other systems (no data).

AN 2004:303255 CAPLUS <<LOGINID::20071212>>
DN 141:54277
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the α2δ subunit of voltage-gated calcium channels
AU Hu, Tao; Stearns, Brian A.; Campbell, Brian T.; Arruda, Jeannie M.; Chen, Chixu; Aiyar, Jayashree; Bezverkov, Robert E.; Santini, Angelina; Schaffhauser, Herve; Liu, Wensheng; Venkatraman, Shankar; Munoz, Benito
CS MRLSDB2, Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2031-2034
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 141:54277
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the α2δ subunit of voltage gated calcium channels
GI

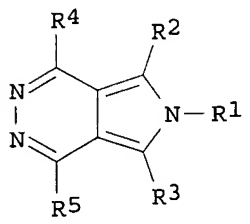


I

AB A novel class of 6-aryl-6H-pyrrolo[3,4-d]pyridazine ligands for the α2δ subunit of voltage-gated calcium channels has been described. Substitutions in the aryl ring of the mol. were generally not tolerated, and resulted in diminished binding to the α2δ subunit. Modifications to the pyridazine ring revealed numerous permissive substitutions, and detailed SAR studies were carried out in this portion of the mol. Replacement of the pyridazine ring Me group with an aminomethyl functionality provided greatly improved potency over the initial lead. The initial lead compound (I) displayed good rat pharmacokinetic properties, and was shown to be efficacious in the Chung model for neuropathic pain in rats.
AN 2004:153601 CAPLUS <<LOGINID::20071212>>
DN 140:357282
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the α2δ subunit of voltage gated calcium channels
AU Stearns, Brian A.; Anker, Naomi; Arruda, Jeannie M.; Campbell, Brian T.; Chen, Chixu; Cramer, Merryl; Hu, Tao; Jiang, Xiaohui; Park, Kenneth; Ren, Kun Kun; Sablad, Marciano; Santini, Angelina; Schaffhauser, Herve; Urban, Mark O.; Munoz, Benito
CS Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1295-1298
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.
DT Journal
LA English
OS CASREACT 140:357282
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds
GI



I

AB The title compds. [I; R1 = (un)substituted alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl; R2-R5 = a bond, (un)substituted alkyl, alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl] were prepared as as ligands of voltage gated calcium channels (VGCC), useful in the treatment of neuropathic pain, and psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson s disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, drug addiction, drug abuse, drug withdrawal and other. E.g., a multi-step synthesis of I [R1 = 4-EtOC6H4; R2-R4 = Me; R5 = 4-MeOC6H4] which produced a 65% effect after i.p. dosing at 30 mg/kg in spinal nerve ligation model of neuropathic pain in rats, was given. The pharmaceutical composition comprising the compound I is claimed.
AN 2004:60243 CAPLUS <<LOGINID::20071212>>
DN 140:111422
TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds
IN Anker, Naomi Burke; Arruda, Jeannie M.; Campbell, Brian Thomas; Munoz, Benito; Prasit, Petpiboon; Stearns, Brian A.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 203 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004006836	A2	20040122	WO 2003-US21493	20030708
WO 2004006836	A3	20040415		

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CA 2492022	A1	20040122	CA 2003-2492022	20030708

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     AU 2003248907         B2     20070426
     EP 1539168            A2     20050615    EP 2003-764414          20030708
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            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
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     US 2006154929         A1     20060713    US 2005-520962          20051128
PRAI US 2002-394734P       P      20020711
     WO 2003-US21493       W      20030708
OS   MARPAT 140:111422

L4   ANSWER 7 OF 7  CAPLUS  COPYRIGHT 2007 ACS on STN
TI   Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-
     d]pyridazines
AB   Dipyrrolo[1,2-b:3,4-d]pyridazines were prepared from 1,4,5,7-tetramethyl-6-
     R1-pyrrolo[3,4-d]-pyridazines.  The dipyrrolo[1,2-b:3,4-d]pyridazines were
     found to have high nucleophilicity and electrophilic substitution occurs
     at C7, or C7 and C9 depending on the steric bulk and activity of the
     attacking electrophile.
AN   2003:927977  CAPLUS <<LOGINID::20071212>>
DN   140:303615
TI   Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-
     d]pyridazines
AU   Arsen'ev, V. G.; Arsen'eva, M. Yu.; Shopin, D. V.; Olekhnovich, L. P.
CS   Rostov State University, Rostov-on-Don, 344006, Russia
SO   Chemistry of Heterocyclic Compounds (New York, NY, United
     States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2003),
     39(5), 669-670
     CODEN: CHCCAL; ISSN: 0009-3122
PB   Kluwer Academic/Consultants Bureau
DT   Journal
LA   English
OS   CASREACT 140:303615
RE.CNT  4     THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT


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L4           7 S L3

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FULL ESTIMATED COST                                   20.28     193.94

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CA SUBSCRIBER PRICE                                   -5.46      -5.46

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:21:37 ON 12 DEC 2007

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Welcome to STN International! Enter x:x

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PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
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FILE 'CAPLUS' ENTERED AT 10:28:35 ON 12 DEC 2007
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FULL ESTIMATED COST	20.28	193.94

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE	-5.46	-5.46

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STRUCTURE FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0
DICTIONARY FILE UPDATES: 11 DEC 2007 HIGHEST RN 957570-32-0

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http://www.cas.org/support/stngen/stndoc/properties.html

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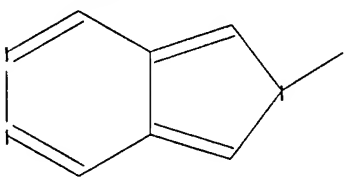

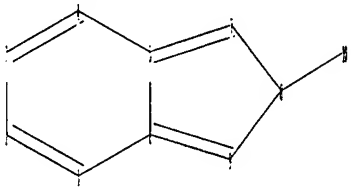

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ring nodes :
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ring bonds :
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exact/norm bonds :
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G1:H,Cy

Match level :
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BATCH **COMPLETE**
PROJECTED ITERATIONS: 117239 TO 126601
PROJECTED ANSWERS: 1 TO 164

L6 1 SEA SSS SAM L5

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L6 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazinium, 1-ethoxy-2,5,6,7-tetramethyl-, tetrafluoroborate(1-) (9CI)
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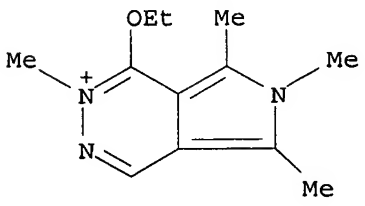

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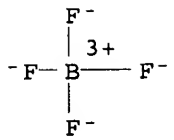

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100.0% PROCESSED 120189 ITERATIONS 86 ANSWERS
SEARCH TIME: 00.00.01

L7 86 SEA SSS FUL L5

=> file caplus

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FULL ESTIMATED COST	172.10	366.04

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CA SUBSCRIBER PRICE	0.00	-5.46

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FILE COVERS 1907 - 12 Dec 2007 VOL 147 ISS 25
FILE LAST UPDATED: 11 Dec 2007 (20071211/ED)

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http://www.cas.org/infopolicy.html

=> s l7
L8 19 L7

=> d l8 1-19 ti abs bib hitstr

L8 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles
AB A small library of 2-oxo-5-(hetero)arylpyrroles was prepared starting from 2,3-dioxo-5-(hetero)arylpyrrolidines. The large synthetic possibilities

of these 2-oxopyrroles were investigated. The 2-oxopyrroles offer a large number of possible derivatizations including reactions with electrophiles. The chloroformylation of 2-oxo-5-(hetero)arylpyrroles provides pyrrole carbaldehydes. Some pyrrole carbaldehydes were used to synthesize polycyclic compds. like pyrrolo[3,4-d]pyridazinones, a thienopyrrole, a pyrrolobenz[1,4]oxazepine, a pyrrolobenzo[1,4]thiazepine, and a pyrrolobenzo[1,4]diazepine. Hereby we showed through a short exploration that the oxopyrroles and analogs are interesting and versatile synthetic building blocks.

AN 2006:498781 CAPLUS <<LOGINID::20071212>>
DN 145:167033
TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles
AU Metten, Bert; Kostermans, Maarten; Van Baelen, Gitte; Smet, Mario; Dehaen, Wim
CS Department of Chemistry, Katholieke Universiteit Leuven, Louvain, B-3001, Belg.
SO Tetrahedron (2006), 62(25), 6018-6028
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 145:167033
IT 901764-67-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of library of 5-aryl-2-oxopyrrole derivs. from 2,3-dioxo-5-arylpyrrolidines and their use as synthons for highly substituted pyrroles)
RN 901764-67-8 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 5-chloro-2,6-dihydro-7-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

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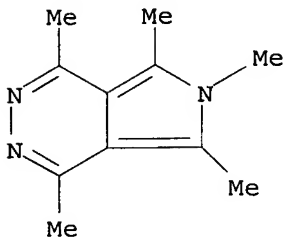
RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

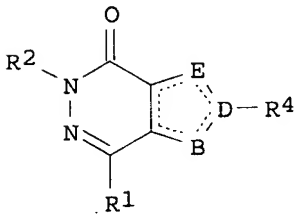
L8 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines
AB Dipyrrolo[1,2-b:3,4-d]pyridazines were prepared from 1,4,5,7-tetramethyl-6-R1-pyrrolo[3,4-d]-pyridazines. The dipyrrolo[1,2-b:3,4-d]pyridazines were found to have high nucleophilicity and electrophilic substitution occurs at C7, or C7 and C9 depending on the steric bulk and activity of the attacking electrophile.
AN 2003:927977 CAPLUS <<LOGINID::20071212>>
DN 140:303615
TI Synthesis and electrophilic substitution of dipyrrolo[1,2-b:3,4-d]pyridazines
AU Arsen'ev, V. G.; Arsen'eva, M. Yu.; Shopin, D. V.; Olekhnovich, L. P.
CS Rostov State University, Rostov-on-Don, 344006, Russia
SO Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2003), 39(5), 669-670
CODEN: CHCCAL; ISSN: 0009-3122
PB Kluwer Academic/Consultants Bureau
DT Journal
LA English
OS CASREACT 140:303615
IT 79398-46-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of dipyrrolopyridazines from pyrrolopyridazines and their reactivity in electrophilic substitution reactions)

RN 79398-46-2 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,6,7-pentamethyl- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN
TI Preparation of novel fused pyridazinones useful as immunosuppressants
GI



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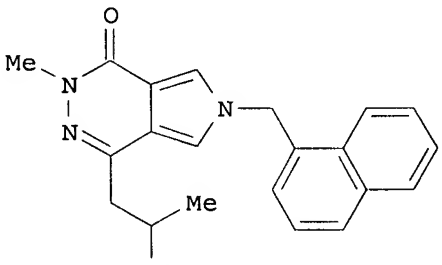

II

AB The invention provides certain pyrrolo-, thieno-, furano- and pyrazolo[3,4-d]pyridazinones of general formula I [B = CH, N, S, or O; D = C or N; E = CR3 or N; with various dependencies; R1 = alkyl, alkoxy, (di)(alkyl)amino, Ph, cycloalkyl, etc.; R2 = Me, alkyl, alkoxyalkyl; R3 = H, (un)substituted carbamoyl, various derivs. of OH and SH; R4 = (un)substituted (hetero)arylmethyl, (hetero)aroyl, (hetero)arylhydroxymethyl, acenaphthenyl, indanyl, or fluorenyl] and their pharmaceutically acceptable salts or solvates. Also disclosed are processes for their preparation, pharmaceutical compns. containing them, a process for preparing the pharmaceutical compns., and methods of treatment involving their use. In particular, their use in immunosuppression, and especially in therapy of reversible obstructive airways diseases, is claimed. For example, title compound II was prepared in 4 steps: (1) bromination of 4-methyl-2-pentanone and reaction with Ph3P:CHCO2Me to give (E)-Me 6-methyl-4-oxo-2-heptenoate; (2) cyclization of the latter with tosylmethyl isocyanide in DMSO to give a pyrrole derivative; (3) N-alkylation of the pyrrole using NaH and 1-naphthalenylmethyl chloride in DMF; and (4) cyclocondensation of the pyrrole sidechains with methylhydrazine. As inhibitors of human mixed lymphocyte reaction in vitro, the example compds. had IA50 values of < 1 + 10-6 M.
AN 1999:388188 CAPLUS <<LOGINID::20071212>>
DN 131:44836
TI Preparation of novel fused pyridazinones useful as immunosuppressants

IN Bantick, John; Cooper, Martin; Thorne, Philip; Perry, Matthew
PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag
SO PCT Int. Appl., 94 pp.
    CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9929695	A1	19990617	WO 1998-SE2191	19981201
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	US 6342601	B1	20020129	US 1999-214755	19990112
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	US 6770646	B2	20040803		
	US 2004162410	A1	20040819	US 2004-776245	20040212
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	SE 1996-556	A	19960215		
	WO 1996-SE1680	W	19961217		

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L9   18 L8 NOT L4

=> d l9 1-18 ti abs bib hitstr

L9 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly substituted pyrroles
AB A small library of 2-oxo-5-(hetero)arylpyrroles was prepared starting from 2,3-dioxo-5-(hetero)arylpyrrolidines. The large synthetic possibilities of these 2-oxopyrroles were investigated. The 2-oxopyrroles offer a large number of possible derivatizations including reactions with electrophiles. The chloroformylation of 2-oxo-5-(hetero)arylpyrroles provides pyrrole carbaldehydes. Some pyrrole carbaldehydes were used to synthesize polycyclic compds. like pyrrolo[3,4-d]pyridazinones, a thienopyrrole, a pyrrolobenz[1,4]oxazepine, a pyrrolobenzo[1,4]thiazepine, and a pyrrolobenzo[1,4]diazepine. Hereby we showed through a short exploration that the oxopyrroles and analogs are interesting and versatile synthetic building blocks.
AN 2006:498781 CAPLUS <<LOGINID::20071212>>
DN 145:167033
TI Synthesis of 5-aryl-2-oxopyrrole derivatives as synthons for highly

substituted pyrroles

AU Metten, Bert; Kostermans, Maarten; Van Baelen, Gitte; Smet, Mario; Dehaen, Wim

CS Department of Chemistry, Katholieke Universiteit Leuven, Louvain, B-3001, Belg.

SO Tetrahedron (2006), 62(25), 6018-6028
CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier B.V.

DT Journal

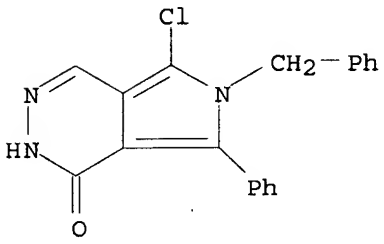
LA English

OS CASREACT 145:167033

IT 901764-67-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of library of 5-aryl-2-oxopyrrole derivs. from 2,3-dioxo-5-arylpyrrolidines and their use as synthons for highly substituted pyrroles)

RN 901764-67-8 CAPLUS

CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 5-chloro-2,6-dihydro-7-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

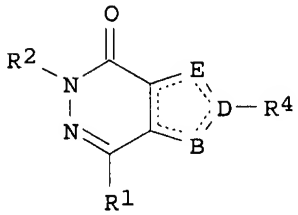


RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Preparation of novel fused pyridazinones useful as immunosuppressants

GI



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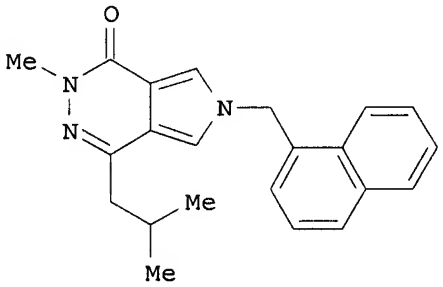

II

AB The invention provides certain pyrrolo-, thieno-, furano- and pyrazolo[3,4-d]pyridazinones of general formula I [B = CH, N, S, or O; D = C or N; E = CR3 or N; with various dependencies; R1 = alkyl, alkoxy, (di)(alkyl)amino, Ph, cycloalkyl, etc.; R2 = Me, alkyl, alkoxyalkyl; R3 = H, (un)substituted carbamoyl, various derivs. of OH and SH; R4 = (un)substituted (hetero)arylmethyl, (hetero)aroyl, (hetero)arylhydroxymethyl, acenaphthenyl, indanyl, or fluorenyl] and their

pharmaceutically acceptable salts or solvates. Also disclosed are processes for their preparation, pharmaceutical compns. containing them, a process for preparing the pharmaceutical compns., and methods of treatment involving their use. In particular, their use in immunosuppression, and especially in therapy of reversible obstructive airways diseases, is claimed. For example, title compound II was prepared in 4 steps: (1) bromination of 4-methyl-2-pentanone and reaction with Ph3P:CHCO2Me to give (E)-Me 6-methyl-4-oxo-2-heptenoate; (2) cyclization of the latter with tosylmethyl isocyanide in DMSO to give a pyrrole derivative; (3) N-alkylation of the pyrrole using NaH and 1-naphthalenylmethyl chloride in DMF; and (4) cyclocondensation of the pyrrole sidechains with methylhydrazine. As inhibitors of human mixed lymphocyte reaction in vitro, the example compds. had IA50 values of < 1 + 10-6 M.

AN 1999:388188 CAPLUS <<LOGINID::20071212>>

DN 131:44836

TI Preparation of novel fused pyridazinones useful as immunosuppressants

IN Bantick, John; Cooper, Martin; Thorne, Philip; Perry, Matthew

PA Astra Pharmaceuticals Ltd., UK; Astra Aktiebolag

SO PCT Int. Appl., 94 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9929695	A1	19990617	WO 1998-SE2191	19981201
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2312419	A1	19990617	CA 1998-2312419	19981201
	AU 9917916	A	19990628	AU 1999-17916	19981201
	EP 1036076	A1	20000920	EP 1998-962754	19981201
	EP 1036076	B1	20020904		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 9813373	A	20001003	BR 1998-13373	19981201
	TR 200001603	T2	20001023	TR 2000-1603	19981201
	EE 200000318	A	20010815	EE 2000-318	19981201
	HU 2001000280	A2	20011028	HU 2001-280	19981201
	HU 2001000280	A3	20030328		
	JP 2001525413	T	20011211	JP 2000-524288	19981201
	NZ 504452	A	20020531	NZ 1998-504452	19981201
	AT 223413	T	20020915	AT 1998-962754	19981201
	US 6342601	B1	20020129	US 1999-214755	19990112
	NO 2000002788	A	20000801	NO 2000-2788	20000531
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	US 6770646	B2	20040803		
	US 2004162410	A1	20040819	US 2004-776245	20040212
PRAI	SE 1997-4542	A	19971205		
	SE 1998-1989	A	19980604		
	GB 1995-26273	A	19951221		
	SE 1996-556	A	19960215		
	WO 1996-SE1680	W	19961217		
	US 1997-776231	A1	19970131		
	WO 1998-SE2191	W	19981201		
	US 1999-214755	A3	19990112		
	US 1999-353644	A1	19990715		
	US 2000-708449	B1	20001109		

US 2002-74008 B1 20020214
OS MARPAT 131:44836
IT 227321-70-2P, 2,6-Dihydro-4-(2-methylpropyl)-6-(1-naphthalenylmethyl)-1H-pyrrolo[3,4-d]pyridazin-1-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fused pyridazinones as immunosuppressants)
RN 227321-70-2 CAPLUS
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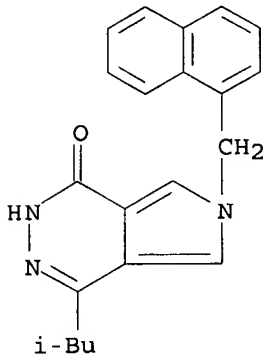

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Investigation of the structure of and the properties of the potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in the gaseous and aqueous phases using the AM1 semi-empirical method
AB Potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones and their fixed tautomeric forms have been studied in order to predict their tautomeric equilibrium consts. and pKa values using semi-empirical AM1 quantum-chemical calcns. at the SCF level in the gas phase and in aqueous solution Hydroxy-oxo forms were found to be more stable than dioxo and dihydroxy forms. The results obtained from the tautomeric equilibrium and basicity calcns. are in good agreement with exptl. data.
AN 1998:451319 CAPLUS <<LOGINID::20071212>>
DN 129:175315
TI Investigation of the structure of and the properties of the potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in the gaseous and aqueous phases using the AM1 semi-empirical method
AU Guven, Alaattin; Ogretir, Cemil
CS Faculty of Science, Chemistry Department, Anadolu University, Eskiehir, Turk.
SO THEOCHEM (1998), 434, 7-28
CODEN: THEODJ; ISSN: 0166-1280
PB Elsevier Science B.V.
DT Journal
LA English
IT 96441-75-7 96441-82-6 211247-93-7
211247-94-8 211248-10-1 211389-39-8
211450-67-8
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(structure of and properties of potentially tautomeric 1,2,3,4-tetrahydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in gaseous and aqueous phases using AM1)

RN 96441-75-7 CAPLUS
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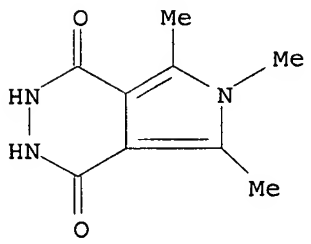
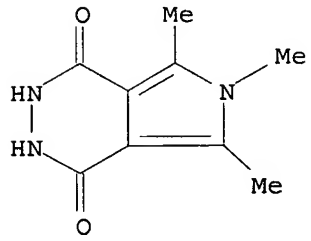
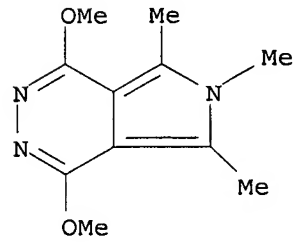


RN 96441-82-6 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)

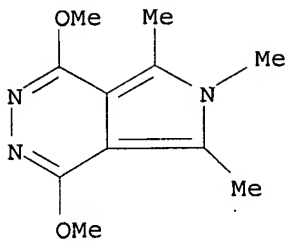


● H^+

RN 211247-93-7 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dimethoxy-5,6,7-trimethyl- (CA INDEX NAME)

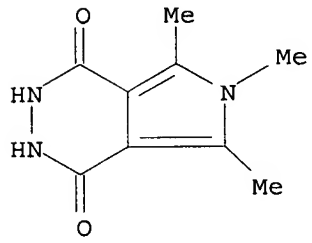


RN 211247-94-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dimethoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



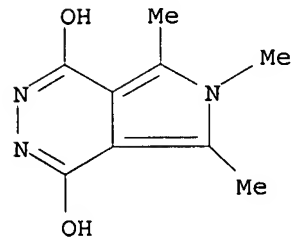
● H^+

RN 211248-10-1 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)

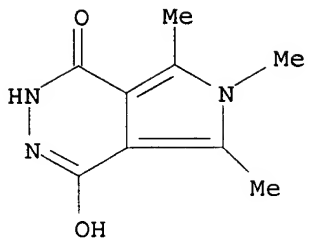


● 2 H^+

RN 211389-39-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 5,6,7-trimethyl- (CA INDEX NAME)

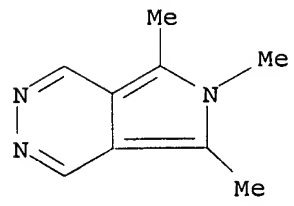


RN 211450-67-8 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-4-hydroxy-5,6,7-trimethyl- (CA INDEX NAME)

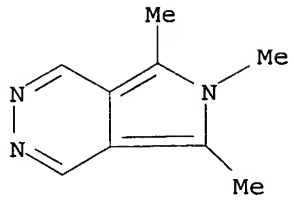


RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Investigation of the structure and properties of the potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in the gas and aqueous phases using the AM1 and PM3/COSMO solvation method
AB The potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines, 2H and 6H, and their fixed tautomeric forms were studied in order to predict the most stable form by the restricted Hartree-Foch approach using semiempirical PM3 and AM1 quantum chemical calcns. at the SCF level in the gas and aqueous phases. Both methods predicted that the 6H form is more stable than the other forms in both gas and aqueous phases. The results obtained were found to be in agreement with the exptl. data. Monoprotonated forms of 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines were also examined Proton affinity calcns. predicted that the first protonations take place on the N6 atom in the 2H form and on the N2 atom in the 6H form, resulting in a common cation.
AN 1998:220258 CAPLUS <<LOGINID::20071212>>
DN 128:321258
TI Investigation of the structure and properties of the potentially tautomeric 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in the gas and aqueous phases using the AM1 and PM3/COSMO solvation method
AU Guven, Alaattin; Ogretir, Cemil
CS Fac. Sci., Chem. Dep., Anadolu Univ., Eskisehir, Turk.
SO THEOCHEM (1998), 430, 85-95
CODEN: THEODJ; ISSN: 0166-1280
PB Elsevier Science B.V.
DT Journal
LA English
IT 30476-58-5 206860-75-5 206860-78-8
RL: PRP (Properties)
(AM1 and PM3/COSMO solvation method in study of tautomeric nature of 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines in gas and aqueous phases)
RN 30476-58-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)

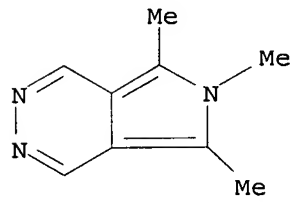


RN 206860-75-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



● H^+

RN 206860-78-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)

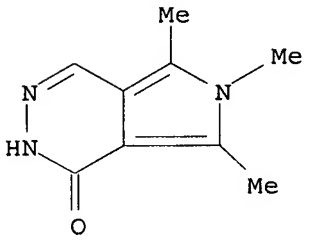


●2 H^+

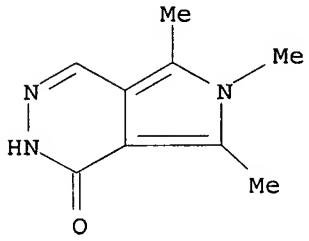
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Investigation of the structure and the properties of the potentially tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in the gas and aqueous phases using semiempirical methods
AB Potentially tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones and their fixed tautomeric forms have been studied, in order to predict their tautomeric equilibrium consts. and pKa values, using semiempirical PM3, AM1 quantum-chemical calcns. at the SCF level in the gas phase and in aqueous solution The effect of alkylation on the pKa value was also investigated. In both the gas phase and in aqueous solution, oxo forms have been found to be more stable than hydroxy and zwitterionic structures. The results obtained from the tautomeric equilibrium and acidity calcns. are in good agreement with exptl. data.
AN 1998:199391 CAPLUS <<LOGINID::20071212>>
DN 129:4401
TI Investigation of the structure and the properties of the potentially tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in the gas and aqueous phases using semiempirical methods
AU Guven, Alaatin; Ogretir, Cemil
CS Fac. Sci., Chem. Dep., Anadolu Univ., Eskisehir, Turk.
SO THEOCHEM (1998), 427, 65-77
CODEN: THEODJ; ISSN: 0166-1280
PB Elsevier Science B.V.

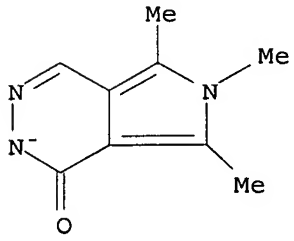
DT Journal
LA English
IT 90817-87-1 96441-64-4 207286-20-2
207286-21-3 207286-22-4 207286-23-5
207286-24-6 207286-25-7 207286-26-8
207355-02-0 207355-03-1 207355-04-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(structure and properties of potentially tautomeric 1,2-dihydro-5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazine-1-ones in gas and aqueous phases using semiempirical methods)
RN 90817-87-1 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX NAME)



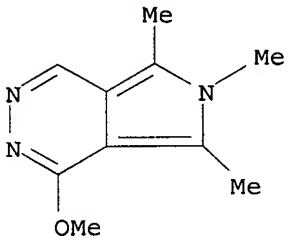
RN 96441-64-4 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



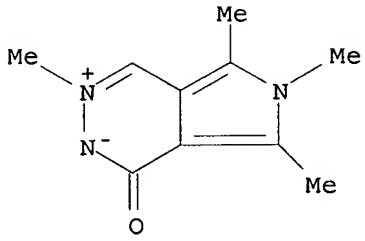
RN 207286-20-2 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, ion(1-) (CA INDEX NAME)



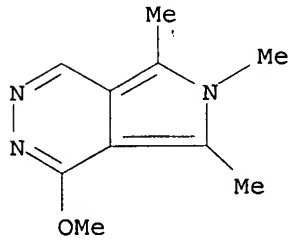
RN 207286-21-3 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-methoxy-5,6,7-trimethyl- (CA INDEX NAME)



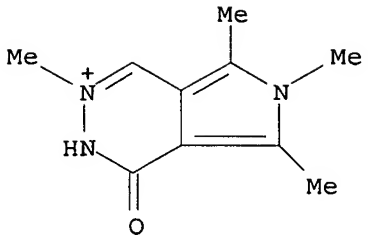
RN 207286-22-4 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazinium, 2,6-dihydro-3,5,6,7-tetramethyl-1-oxo-, inner salt (CA INDEX NAME)



RN 207286-23-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-methoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



RN 207286-24-6 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazinium, 2,6-dihydro-3,5,6,7-tetramethyl-1-oxo- (CA INDEX NAME)



RN 207286-25-7 CAPLUS
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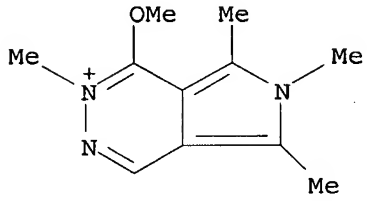
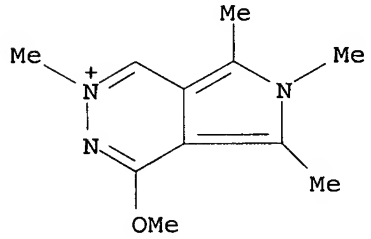
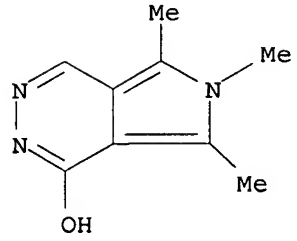


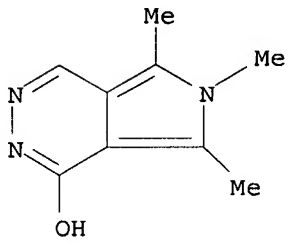
RN 207286-26-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-methoxy-2,5,6,7-tetramethyl- (CA INDEX NAME)



RN 207355-02-0 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)

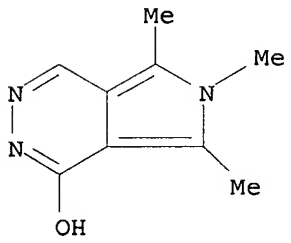


RN 207355-03-1 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)



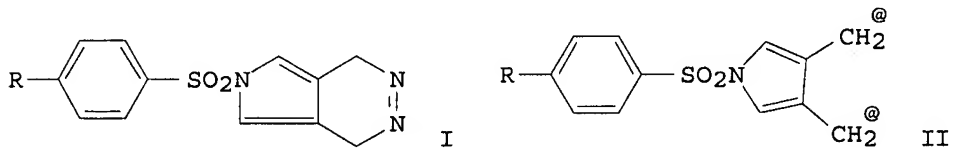
●2 H^+

RN 207355-04-2 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazin-1-ol, 5,6,7-trimethyl- (CA INDEX NAME)



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

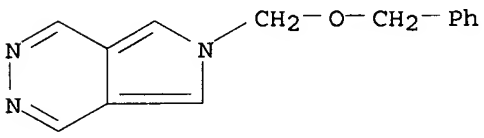
L9 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Long-lived spin isomerism of singlet and triplet states of N-arenesulfonyl-3,4-dimethylenepyrroles
GI



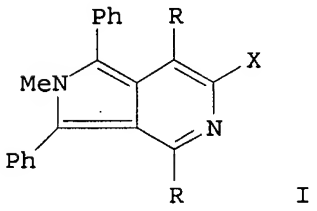
AB A theor. prediction that attachment of an electron-withdrawing group to the ring nitrogen of a 3,4-dimethylenepyrrole biradical should selectively stabilize the triplet state is tested by generation of matrix-immobilized transient species in the irradiation of 1,4-dihydro-6-arenesulfonylpyrrolo[3,4-d]pyridazine precursors (I; R = Me, Br) at 265 nm. ESR spectra of triplet species assigned to the corresponding dimethylenepyrroles (II) are observed in both cases. The zero-field splitting parameter D is 0.023 cm-1 in both cases, essentially the same as those reported in the literature for

tetramethyleneethane derivs. Irradiation of the precursors at 370 nm gives rise in both cases to the corresponding singlets, blue (λmax 593 and 600 nm, resp.), ESR-silent substances. The spin isomers do not interconvert over a period of days.

AN 1994:133629 CAPLUS <<LOGINID::20071212>>
DN 120:133629
TI Long-lived spin isomerism of singlet and triplet states of N-arenesulfonyl-3,4-dimethylenepyrroles
AU Bush, Linda C.; Heath, Richard B.; Berson, Jerome A.
CS Dep. Chem., Yale Univ., New Haven, CT, 06511, USA
SO Journal of the American Chemical Society (1993), 115(21), 9830-1
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
IT 152940-60-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 152940-60-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 6-[(phenylmethoxy)methyl]- (CA INDEX NAME)



L9 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Substituent effects on the spectra of fluorescent aryl-substituted N-methylpyrrolo[3,4-c]pyridines
GI

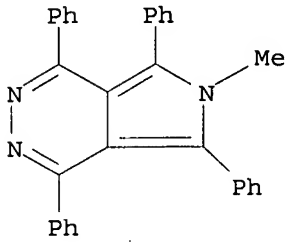


I

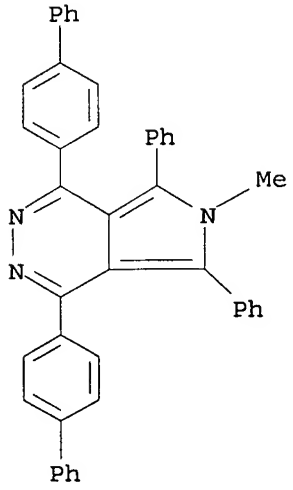
AB Introduction of an alkoxy group into the Ph ring at the 4 and 7 positions of I (R = aryl; X = CN, CONH2, CO2H) had little effect on the absorption and emission spectra of the title dyes, while introduction of a Br group caused a red shift in the spectrum of I (X = CN). I (X = CN, CO2Et, H) were strongly fluorescent, while the fluorescence of I (X = CONH2) was weak; I (X = CONHNH2, CO2H) were also weakly fluorescent with a large Stokes shift (.apprx.150 nm). Related pyridazines were not fluorescent.

AN 1993:82819 CAPLUS <<LOGINID::20071212>>
DN 118:82819
TI Substituent effects on the spectra of fluorescent aryl-substituted N-methylpyrrolo[3,4-c]pyridines
AU Mataka, Shuntaro; Tashiro, Masashi; Misumi, Osamu; Lin, Wei Hua; Takahashi, Kazufumi; Torii, Akiyoshi
CS Inst. Adv. Mater. Study, Kyushu Univ., Kasuga, 816, Japan
SO Dyes and Pigments (1992), 20(2), 83-96
CODEN: DYPIDX; ISSN: 0143-7208

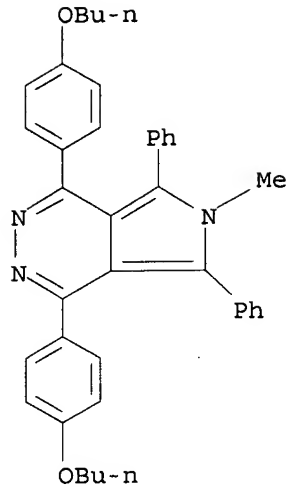
DT Journal
LA English
IT 145551-53-7P 145551-54-8P 145551-55-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and fluorescence of, substituent effect in relation to)
RN 145551-53-7 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 6-methyl-1,4,5,7-tetraphenyl- (CA INDEX NAME)



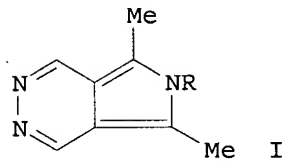
RN 145551-54-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-bis([1,1'-biphenyl]-4-yl)-6-methyl-5,7-diphenyl- (CA INDEX NAME)



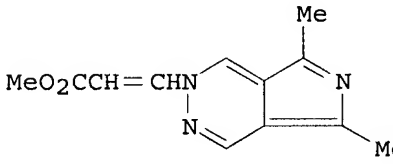
RN 145551-55-9 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-bis(4-butoxyphenyl)-6-methyl-5,7-diphenyl- (CA INDEX NAME)



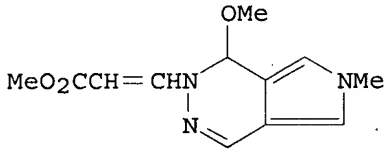
L9 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Pyrrole studies. Part 39. The disparate reactivity of 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines with acetylenic esters and with azodicarboxylic esters
GI



I



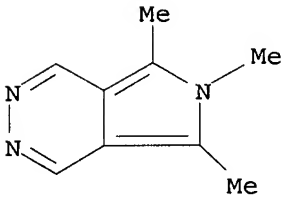
II



III

AB Reaction of MeO2CC.tplbond.CH with the title pyrrolopyridazines I (R = H, Me) in MeOH gave adducts II and III, resp., but no ring opened products. In contrast, EtO2CN:NCO2Et underwent reaction with I (R = H) at the electron-rich 5-membered ring.
AN 1988:510358 CAPLUS <<LOGINID::20071212>>
DN 109:110358
TI Pyrrole studies. Part 39. The disparate reactivity of 5,7-dimethyl-6H-pyrrolo[3,4-d]pyridazines with acetylenic esters and with azodicarboxylic esters
AU Fuentes Rodriguez, Fernanda; Sepulveda-Arques, Jose; Jones, R. Alan
CS Fac. Farm., Univ. Valencia, Valencia, 46010, Spain
SO Journal of Chemical Research, Synopses (1987), (11), 356
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English
OS CASREACT 109:110358
IT 30476-58-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with Me propiolate)
RN 30476-58-5 CAPLUS

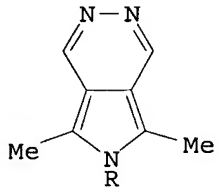
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



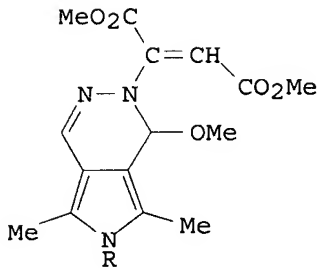
L9 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN

TI Pyrrole studies. Part 32. A novel ring-cleavage reaction of the pyridazine ring during the reaction of 6H-pyrrolo[3,4-d]pyridazines with dimethyl acetylenedicarboxylate

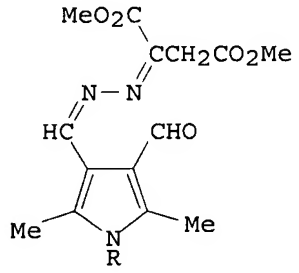
GI



I



II



III

AB Treatment of pyrrolopyridazines I (R = Me, H, Ph) with (MeO2CC.tplbond.)2 in MeOH at -70° gave the corresponding esters II (R as before), which were unstable in the presence of H2O and underwent ring cleavage to the corresponding pyrroles III. The structure of III (R = H) was confirmed by x-ray anal.

AN 1985:471267 CAPLUS <<LOGINID::20071212>>

DN 103:71267

TI Pyrrole studies. Part 32. A novel ring-cleavage reaction of the pyridazine ring during the reaction of 6H-pyrrolo[3,4-d]pyridazines with dimethyl acetylenedicarboxylate

AU Hernandez de la Figuera Gomez, Teresa; Sepulveda Arques, Jose; Jones, R. Alan; Dawes, Helen M.; Hursthouse, Michael B.

CS Dep. Quim. Org., Univ. Valencia, Valencia, Spain

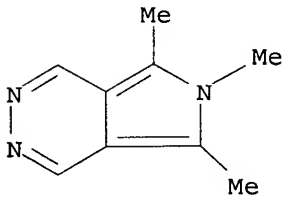
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (4), 899-902
CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

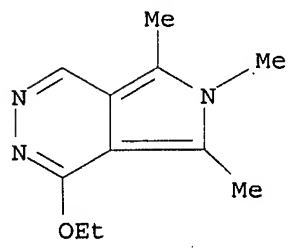
LA English

OS CASREACT 103:71267

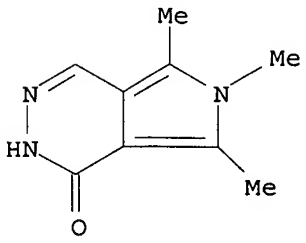
IT 30476-58-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with di-Me acetylenedicarboxylate)
RN 30476-58-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Pyrrole studies: 31. The structures of potentially tautomeric 1,2-dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones and 1,2,3,4-tetrahydro-6H-pyrrolo[3,4-d]pyridazine-1,4-diones
AB 1,2-Dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones exist predominantly as such in equilibrium with the 1-hydroxypyridazine form, whereas 1,2,3,4-tetrahydro-6H-pyrrolo[3,4-d]pyridazine-1,4-diones in equilibrium with the monohydroxy-oxo tautomeric forms are preferred by a factor of only .apprx.100:1. It was not possible to determine the position of equilibrium between the 1-hydroxy-6H-pyrrolo[3,4-d]pyridazin-4-one and the 1,4-dihydroxy-6H-pyrrolo[3,4-d]pyridazine structures.
AN 1985:422083 CAPLUS <<LOGINID::20071212>>
DN 103:22083
TI Pyrrole studies: 31. The structures of potentially tautomeric 1,2-dihydro-6H-pyrrolo[3,4-d]pyridazin-1-ones and 1,2,3,4-tetrahydro-6H-pyrrolo[3,4-d]pyridazine-1,4-diones
AU Inel, Sermin; Jones, R. Alan; Ogretir, Cemil
CS Sch. Chem. Sci., Univ. East Anglia, Norwich, NR4 7TJ, UK
SO Tetrahedron (1984), 40(20), 3979-86
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
OS CASREACT 103:22083
IT 96441-62-2 96441-64-4 96441-67-7
96441-69-9 96441-72-4 96441-73-5
96441-80-4 96441-82-6 96441-86-0
96441-88-2
RL: PRP (Properties)
(UV spectrum of)
RN 96441-62-2 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl- (CA INDEX NAME)

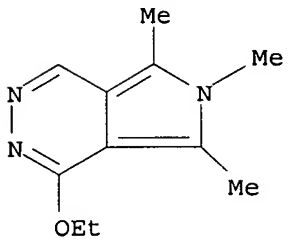


RN 96441-64-4 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



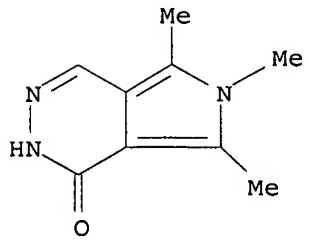
● H^+

RN 96441-67-7 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



● H^+

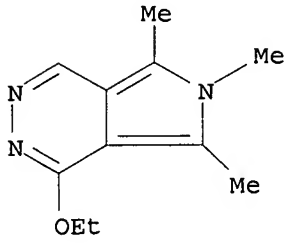
RN 96441-69-9 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)



●2 H^+

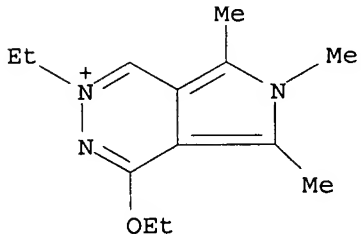
RN 96441-72-4 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 1-ethoxy-5,6,7-trimethyl-, conjugate diacid (9CI) (CA INDEX NAME)



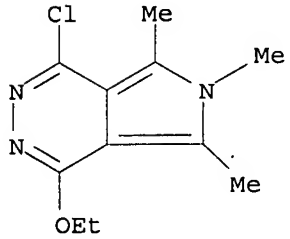
● 2 H^+

RN 96441-73-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-ethoxy-2-ethyl-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)

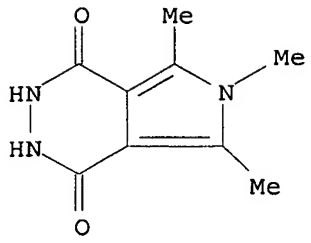


● H^+

RN 96441-80-4 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-4-ethoxy-5,6,7-trimethyl- (CA INDEX NAME)

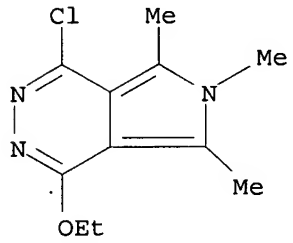


RN 96441-82-6 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)



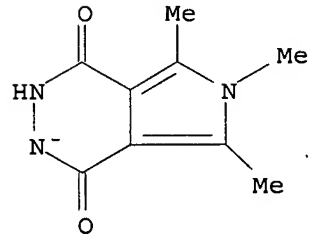
● H^+

RN 96441-86-0 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-4-ethoxy-5,6,7-trimethyl-, conjugate monoacid (9CI) (CA INDEX NAME)

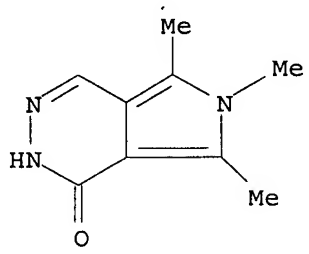


● H^+

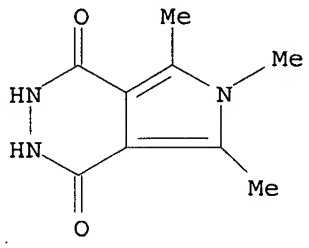
RN 96441-88-2 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl-, ion(1-) (CA INDEX NAME)



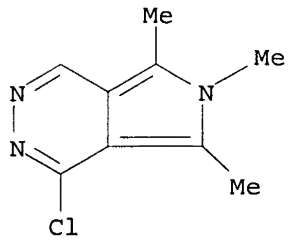
IT 90817-87-1 96441-75-7
RL: PRP (Properties)
(UV spectrum of, absence of tautomerism in relation to)
RN 90817-87-1 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX NAME)



RN 96441-75-7 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 2,3-dihydro-5,6,7-trimethyl- (CA INDEX NAME)

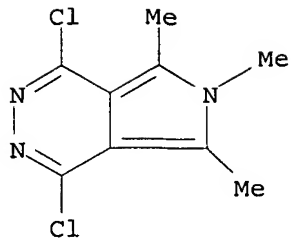


IT 96441-91-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with sodium methoxide)
RN 96441-91-7 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-5,6,7-trimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

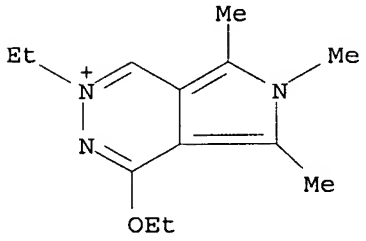
IT 96441-92-8P 96452-45-8P 96452-47-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 96441-92-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4-dichloro-5,6,7-trimethyl- (CA INDEX NAME)



RN 96452-45-8 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 4-ethoxy-2-ethyl-5,6,7-trimethyl-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

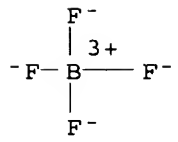
CM 1

CRN 96452-44-7
CMF C13 H20 N3 O



CM 2

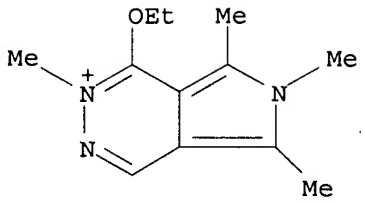
CRN 14874-70-5
CMF B F4
CCI CCS



RN 96452-47-0 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 1-ethoxy-2,5,6,7-tetramethyl-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

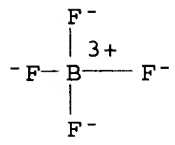
CM 1

CRN 96452-46-9
CMF C12 H18 N3 O

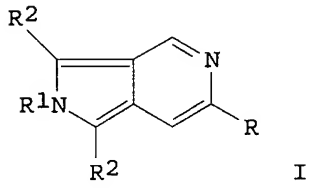


CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



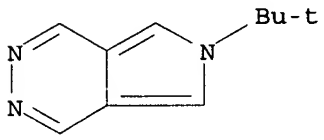
L9 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Structure and reactivity of iso-fused heterocyclic systems with 4n π and (4n + 2) π electrons. 8. Cyclizing condensation of 1H-pyrrole-3,4-dicarbaldehydes with 1,2-bifunctional compounds. A general and simple preparation method for 2H-pyrrolo[3,4-c]pyridines and 6H-pyrrolo[3,4-d]pyridazines
GI



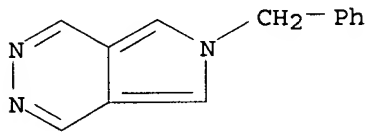
I

AB 2H-Pyrrolo[3,4-c]pyridines I (R = CO2Me, CO2Et, cyano; R1 = H, Me, CMe3, CH2Ph; R2 = H, Me) are easily and efficiently accessible via reaction of 1H-pyrrole-3,4-dicarbaldehydes with H2NCH2R.HCl. Under the influence of Et2NH the cyclocondensation occurs in an uniform fashion and in 55-99% yields. In a similar manner 1H-pyrrole-3,4-dicarbaldehydes react with N2H4; two-fold elimination of H2O leads to 6H-pyrrolo[3,4-d]pyridazines. The bicyclic hetarenes are stabilized compared with 2H-isoindoles by addnl. heteroatoms in the 6-membered ring and acceptor groups at the 6-position.
AN 1985:45802 CAPLUS <<LOGINID::20071212>>
DN 102:45802
TI Structure and reactivity of iso-fused heterocyclic systems with 4n π and (4n + 2) π electrons. 8. Cyclizing condensation of 1H-pyrrole-3,4-dicarbaldehydes with 1,2-bifunctional compounds. A general and simple preparation method for 2H-pyrrolo[3,4-c]pyridines and 6H-pyrrolo[3,4-d]pyridazines
AU Kreher, Richard P.; Pfister, Juergen

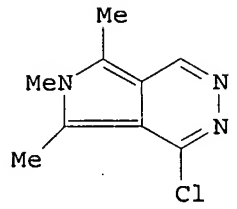
CS Abt. Chem., Univ. Dortmund, Dortmund, D-4600/50, Fed. Rep. Ger.
SO Chemiker-Zeitung (1984), 108(9), 275-7
CODEN: CMKZAT; ISSN: 0009-2894
DT Journal
LA German
OS CASREACT 102:45802
IT 94169-85-4P 94169-86-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 94169-85-4 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 6-(1,1-dimethylethyl)- (CA INDEX NAME)



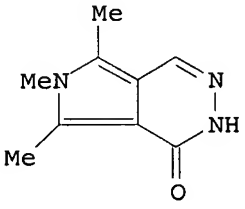
RN 94169-86-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 6-(phenylmethyl)- (CA INDEX NAME)



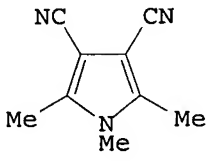
L9 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Pyrrole studies. XXIX. An unusual pyridazine ring-opening reaction
GI



I



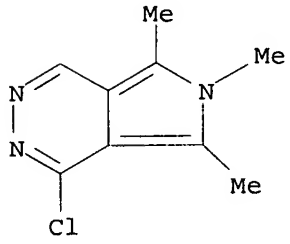
II



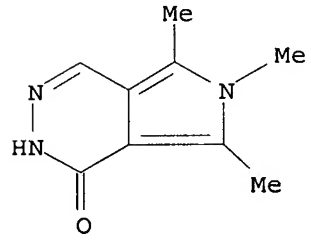
III

AB Treating 1-chloro-5,6,7-trimethylpyrrolo[3,4-d]pyridazine (I) with aqueous or alc. NaOH, NaOEt, or NaOPh gave .apprx.60% pyridazinone II. Treating I with NaOMe in DMF gave 42% dicyanopyrrole III and 40% II; NaOEt in DMF gave 19% III.
AN 1984:423418 CAPLUS <<LOGINID::20071212>>
DN 101:23418
TI Pyrrole studies. XXIX. An unusual pyridazine ring-opening reaction
AU Jones, R. Alan; Inel, Sermin
CS Sch. Chem. Sci., Univ. East Anglia, Norwich, NR4 7TJ, UK
SO Chemistry & Industry (London, United Kingdom) (1984), (7), 270-1
CODEN: CHINAG; ISSN: 0009-3068
DT Journal
LA English
OS CASREACT 101:23418

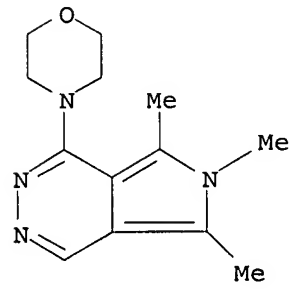
IT 90817-88-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(base-catalyzed ring cleavage of)
RN 90817-88-2 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1-chloro-5,6,7-trimethyl- (CA INDEX NAME)



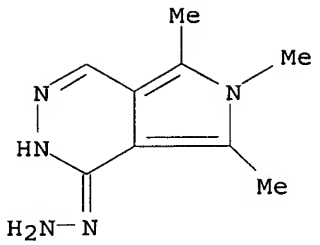
IT 90817-87-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in ring cleavage of chlorotrimethylpyrrolopyridazine)
RN 90817-87-1 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl- (CA INDEX NAME)



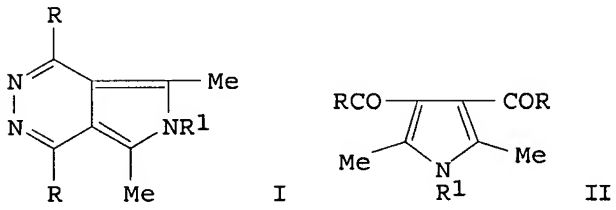
IT 90817-90-6P 90817-91-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 90817-90-6 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl-1-(4-morpholinyl)- (CA INDEX NAME)



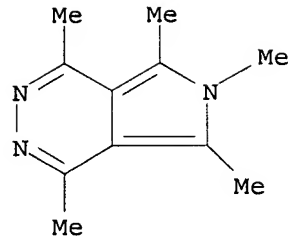
RN 90817-91-7 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazin-1-one, 2,6-dihydro-5,6,7-trimethyl-, hydrazone (9CI) (CA INDEX NAME)



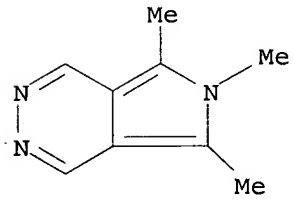
L9 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Pyrrole studies. XXV. Structure of potentially tautomeric pyrrolo[3,4-d]pyridazines
GI



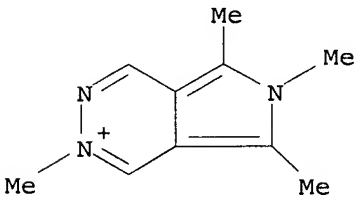
AB Pyrrolopyridazines I (R = H, Me, R1 = H) were prepared by treating the pyrroles II with N2H4. II (R = R1 = H) was obtained by formylating 2,5-dimethylpyrrole and II (R = Me, R1 = H) from Ac2CHCHAc2 and NH4OAc. Methylation gave II (R = H, Me, R1 = Me) which were treated with N2H4 to give I (R = H, Me, R1 = Me). Quaternized derivs. were obtained with MeNHNH2 and MeNHNHMe or by quaternizing I. Electron spectra and basicity measurement showed that I exist in a 6H-form in accordance with MO calcns. of the relative resonance energies of the possible tautomers. Protonation occurs at the heteroatoms and at C-5.
AN 1981:569111 CAPLUS <<LOGINID::20071212>>
DN 95:169111
OREF 95:28269a,28272a
TI Pyrrole studies. XXV. Structure of potentially tautomeric pyrrolo[3,4-d]pyridazines
AU Acar, Fatma; Badesha, Santokh Singh; Flitsch, Wilhelm; Gozogul, Reyhan; Inel, Oguz; Inel, Sermin; Jones, R. Alan; Ogretir, Cemil; Rustidge, David C.
CS Kim. Lab., Devlet Mimarlik Muhendislik Akad., Eskisehir, Turk.
SO Chimica Acta Turcica (1981), 9(1), 225-37
CODEN: CATUA9; ISSN: 0379-5896
DT Journal
LA English
OS CASREACT 95:169111
IT 79398-46-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization of)
RN 79398-46-2 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,6,7-pentamethyl- (CA INDEX NAME)



IT 30476-58-5P 79398-41-7P 79398-43-9P
79398-49-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30476-58-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



RN 79398-41-7 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 2,5,6,7-tetramethyl-, iodide (9CI) (CA INDEX NAME)

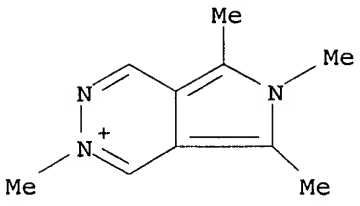


● I^-

RN 79398-43-9 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 2,5,6,7-tetramethyl-, sulfate (1:1) (CA INDEX NAME)

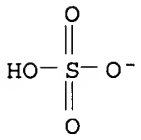
CM 1

CRN 79398-42-8
CMF C10 H14 N3

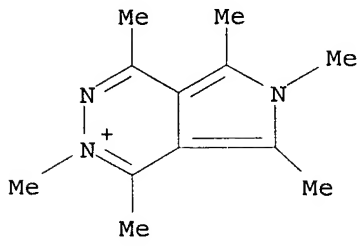


CM 2

CRN 14996-02-2
CMF H O4 S

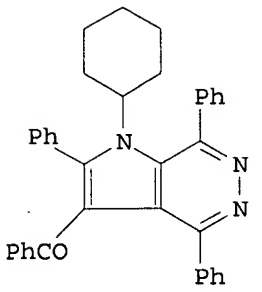


RN 79398-49-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazinium, 1,2,4,5,6,7-hexamethyl-, iodide (9CI) (CA INDEX NAME)

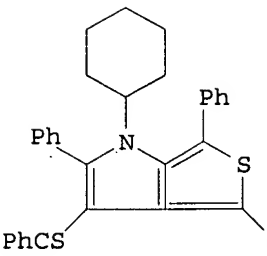


● I^-

L9 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthetic approaches to fused heteroaromatic compounds by the condensation reactions of functional pyrroles
GI



I



II

AB Diacyl- and triacylpyrroles, obtained by one pot synthesis from aziridines and acetylenic dipolarophiles, underwent condensation reactions. On treatment of 3,4-di- and 2,3,4-tribenzoylpyrroles with hydrazine hydrate and phosphorus pentasulfide, pyrrolopyridazine derivs., e.g. I, and fused thiophenes, e.g. II, resp., were prepared The structure proofs for I were based on the 13C FT-NMR spectrum of the corresponding 13C-enriched compds.

AN 1978:443293 CAPLUS <<LOGINID::20071212>>

DN 89:43293

OREF 89:6725a,6728a

TI Synthetic approaches to fused heteroaromatic compounds by the condensation reactions of functional pyrroles

AU Uchida, Takane

CS Fac. Educ., Fukui Univ., Fukui, Japan

SO Journal of Heterocyclic Chemistry (1978), 15(2), 241-8
CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

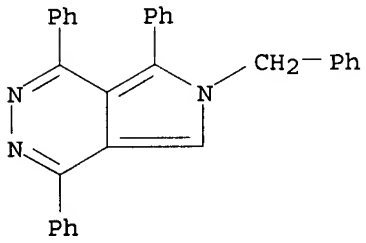
LA English

OS CASREACT 89:43293

IT 66864-43-5P 66864-44-6P 66939-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

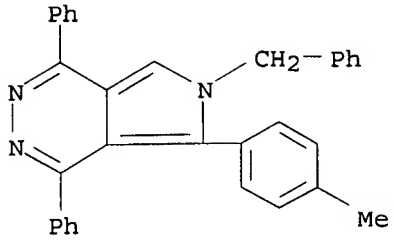
RN 66864-43-5 CAPLUS

CN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5-triphenyl-6-(phenylmethyl)- (CA INDEX NAME)

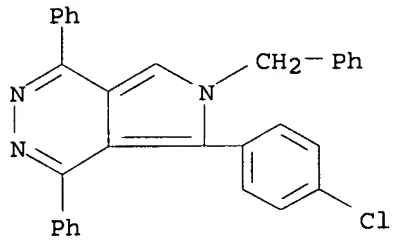


RN 66864-44-6 CAPLUS

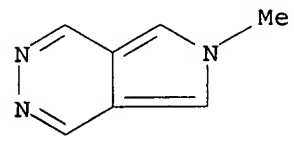
CN 6H-Pyrrolo[3,4-d]pyridazine, 5-(4-methylphenyl)-1,4-diphenyl-6-(phenylmethyl)- (CA INDEX NAME)



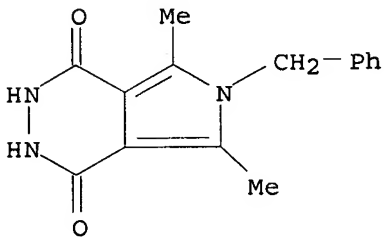
RN 66939-89-7 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5-(4-chlorophenyl)-1,4-dimethyl-6-(phenylmethyl)- (9CI) (CA INDEX NAME)



L9 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis of new condensed pyrrolic heterocycles
GI For diagram(s), see printed CA Issue.
AB 1-Methyl-3,4-diformylpyrrole (I, R = CHO) (prepared by reduction of I (R = CO2Et) to give I (R = CH2OH) followed by oxidation with Ag2CO3) condensed with (MeO2CCH2)2CO, Et2CO, N2H4, and with H2NCH2CO2Et to give the condensed heterocycles II (R = CO2Me and Me) and III (X = N and CCO2Et), resp.
AN 1974:3411 CAPLUS <<LOGINID::20071212>>
DN 80:3411
OREF 80:595a,598a
TI Synthesis of new condensed pyrrolic heterocycles
AU Duflos, J.; Letouze, D.; Queguiner, G.; Pastour, P.
CS Inst. Nat. Super. Chim. Ind., Rouen, Fr.
SO Tetrahedron Letters (1973), (36), 3453-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA French
IT 51110-68-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51110-68-0 CAPLUS
CN 2H-Pyrrolo[3,4-d]pyridazine, 2-methyl- (9CI) (CA INDEX NAME)

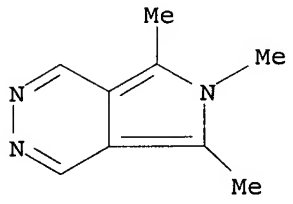


L9 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Syntheses of pyridazino[1,2-a]pyridazine derivatives of furan, pyridazine, and pyrrole by Diels-Alder reactions
GI For diagram(s), see printed CA Issue.
AB Diels-Alder adducts were formed in the Pb(OAc)4 oxidations of substituted cyclic hydrazides of furan, pyridazine, and pyrrole dicarboxylic acids in the presence of 1,3-cyclohexadiene or 1,3-cyclopentadiene. The products resulting were furo[3,4-g]pyridazino[1,2-a]pyridazine-6,10-diones (I), pyridazino[4,5-g]pyridazino[1,2-a]pyridazine-6,11-diones (II), and pyrrolo[3,4-g]pyridazino[1,2-a)pyridazine-6,10-diones (III), resp. Some hydrogenations and ring opening reactions were studied.
AN 1971:99966 CAPLUS <<LOGINID::20071212>>
DN 74:99966
OREF 74:16277a,16280a
TI Syntheses of pyridazino[1,2-a]pyridazine derivatives of furan, pyridazine, and pyrrole by Diels-Alder reactions
AU Gillis, Bernard T.; Valentour, James C.
CS Dep. Chem., Duquesne Univ., Pittsburgh, PA, USA
SO Journal of Heterocyclic Chemistry (1971), 8(1), 13-17
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
IT 31379-83-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31379-83-6 CAPLUS
CN 1H-Pyrrolo[3,4-d]pyridazine-1,4(6H)-dione, 6-benzyl-2,3-dihydro-5,7-dimethyl- (8CI) (CA INDEX NAME)



L9 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Structure and reativity of isocondensed heterocyclic systems with 4n and (4m+2) π-electrons. 2. Cyclizing condensation of 3,4-pyrroledicarboxaldehydes with compounds containing acidic CH and NH groups
GI For diagram(s), see printed CA Issue.
AB 6-Carbethoxy-1,2,3-trimethyl-2H-pyrrolo[3,4-c]-pyridine (I) is prepared by the reaction of 1,2,5-trimethyl-3,4-pyrroledicarboxaldehyde (II) with H2NCH2CO2Et; 1,2,3-trimethyl-2H-pyrrolo[3,4-d]pyridazine (III) is prepared from N2H4. II is treated with RCH2CH2R (R = Bz, CN) to give the corresponding 2H-isoindoles (IV).
AN 1971:53695 CAPLUS <<LOGINID::20071212>>
DN 74:53695
OREF 74:8657a
TI Structure and reativity of isocondensed heterocyclic systems with 4n and (4m+2) π-electrons. 2. Cyclizing condensation of 3,4-pyrroledicarboxaldehydes with compounds containing acidic CH and NH groups
AU Kreher, Richard; Vogt, Guenther
CS Inst. Org. Chem., Tech. Hochsch. Darmstadt, Darmstadt, Fed. Rep. Ger.
SO Angewandte Chemie, International Edition in English (1970), 9(12), 955-6
CODEN: ACIEAY; ISSN: 0570-0833
DT Journal

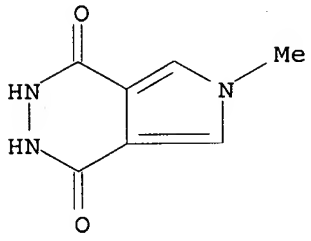
LA English
IT 30476-58-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30476-58-5 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine, 5,6,7-trimethyl- (8CI, 9CI) (CA INDEX NAME)



L9 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2007 ACS on STN
TI Reactions of hydrazine with heterocyclic 1,2-dicarboxylic acid esters
AB The appropriate dicarboxylic acid ester (0.1 mol) in 25-50 cc. MeOH treated with 15 g. $N_2H_4.H_2O$, kept several hrs. at room temperature, heated 0.5 h. on the steam bath, and evaporated, the residue dissolved in 50-500 cc. H_2O containing 5 cc. concentrated NH_4OH, the solution filtered and acidified with excess AcOH or HCl, and the crystalline precipitate washed and dried gave the following condensation products (m.p. and % yield given): 5,8-dihydroxy-1,4,6,7-tetrazanaphthalene (I), 280° (decomposition), 95; 1,3-dimethyl-5,8-dihydroxy-2,6,7-triazanapkthalene, 302° (decomposition), 97; 2-NH_2 derivative of I, above 400°, 93; 2-cyano-3-methyl-5,8-dihydroxy-4,6,7-triazanaphthalene, 320° (decomposition), 85; 2-cyano-3,8-dimethyl-5-hydroxy-4,6,7-triazanaphthalene, 338-40°, 89; 1,4-dimethyl-5,8-dihydroxy-2,3,6,7-tetrazanaphthalene, 320° (decomposition), 73; 4,7-dihydroxy-2-thia-5,6-diazaindene, 328-30°, 92; 2-methyl-4,7-dihydroxy-1-thia-5,6-diazaindene, 294-5°, 90; 1-methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (II), 282-3°, 77; 3-Me derivative of II, 345° (decomposition), 83; 1-phenyl-2-methyl-4,7-dihydroxy-1,5,6-triazaindene, 335-7°, 89; 1-phenyl-4,7-dihydroxy-1,2,5,6-tetrazaindene, 315-16°, 61; 2-mercapto-4,7-dihydroxy-1,3,5,6-tetrazaindene (III), above 400°, 67; 1-methyl-4,7-dihydroxy-1,3,5,6-tetrazaindene, 354-6°, 78°; 1-Me derivative of III, above 330°, 93; 1-phenyl-4,7-dihydroxy-1,3,5,6-tetrazaindene (IV), 315-16°, 89°; 2-SH derivative of IV, 367° (decomposition), 97. The appropriate dicarboxylic dihydrazide (0.05 mol) refluxed 2-8 h. with 50 cc. $N_2H_4.H_2O$ or heated 9-72 h. on the steam bath, the solution evaporated in vacuo on the steam bath, the solid residue dissolved in about 50-200 cc. hot H_2O, and the solution acidified with AcOH or HCl and cooled gave the following condensation products (m.p. and % yield given): 2-methyl-4,7-dihydroxy-1-oxa-5,6-diazaindene (V), 290-2°, 96; 4,7-dihydroxy-2,5,6-triazaindene (VI), above 310°, 90; 2-Me derivative (VII) of VI, 339-40°, 89; 1,5,6-isomer of V, 355° (decomposition), -; 4,7-dihydroxy-1,3,5,6-tetrazaindene (VIII), above 400°, 92. The appropriate dihydrazide (0.05 mol) in 100 cc. 2N HCl heated 6 h. on the steam bath, cooled, and filtered gave the following condensation products: 4,7-dihydroxy-2-oxa-5,6-diazaindene, above 300°, 70; V; VI; VII; VIII. The appropriate diester (0.1 mol) in about 50 cc. MeOH allowed to stand several hrs. with 15 g. $N_2H_4.H_2O$ or heated 0.5 h. on the steam bath, and cooled, and the product recrystd. from H_2O or EtOH or dissolved in dilute acid and repptd. with NH_4OH gave the corresponding dicarboxylic acid dihydrazides (IX) of the following acids (m.p. and % yield of the IX given): 4,5-imidazoledicarboxylic acid, above 375°, 99; 3,4-pyrazoledicarboxylic acid, above 300°, 98;

3,4-furandicarboxylic acid (X), 270° (decomposition), 88; 5-methyl-2,3-furandicarboxylic acid, m. 190°, 94; 3,4-pyrroledicarboxylic acid (XI), above 300°, 95; 1-Me derivative of XI, 330° (decomposition), 90. Dihydrazide of X (16 g.) and 25 cc. N2H4.H2O heated 6 h. on the steam bath, the brown solution evaporated in vacuo, the residue dissolved in 100 cc. dilute aqueous NaOH, and the solution treated with C and acidified with AcOH gave 13 g. 3,3'-dihydroxy-4,4'-bipyrazole (XII), darkened at 360° but did not melt (from H2O); XII was also obtained in 50% yield from di-Et 1-formyl-2-diethoxymethylsuccinate in EtOH with excess N2H4. 1-Methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (XIII) (10 g.) heated 8 h. on the steam bath with 20 cc. N2H4.H2O gave 90% 5-Me derivative of XII, m. above 360° (sublimed at 275° and 0.1 mm.). The 3-Me derivative of XIII gave similarly the 5,5'-di-Me derivative of XII, m. above 375°, in 52% yield when refluxed 15 h. with N2H4.

AN 1956:69457 CAPLUS <<LOGINID::20071212>>
DN 50:69457
OREF 50:13041a-h
TI Reactions of hydrazine with heterocyclic 1,2-dicarboxylic acid esters
AU Jones, Reuben G.
CS Lilly Research Labs., Indianapolis, IN
SO Journal of the American Chemical Society (1956), 78, 159-63
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 50:69457
IT 860362-71-6P, 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 6-methyl-
RL: PREP (Preparation)
(preparation of)
RN 860362-71-6 CAPLUS
CN 6H-Pyrrolo[3,4-d]pyridazine-1,4-diol, 6-methyl- (5CI) (CA INDEX NAME)



=> d his

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L3 237 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:21:22 ON 12 DEC 2007
L4 7 S L3

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L5 STRUCTURE UPLOADED
L6 1 S L5
L7 86 S L5 SSS FULL

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L8             19 S L7
L9             18 S L8 NOT L4

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   112.21     478.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                   -16.38     -21.84

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STN INTERNATIONAL SESSION SUSPENDED AT 10:30:33 ON 12 DEC 2007

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Welcome to STN International!  Enter x:x

LOGINID:SSPTAEXO1623

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 11:31:43 ON 12 DEC 2007
FILE 'CAPLUS' ENTERED AT 11:31:43 ON 12 DEC 2007
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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
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FULL ESTIMATED COST                                   112.21     478.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                   -16.38     -21.84

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FULL ESTIMATED COST                                   113.15     479.19

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CA SUBSCRIBER PRICE                                   -16.38     -21.84

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DICTIONARY FILE UPDATES:  11 DEC 2007  HIGHEST RN 957570-32-0

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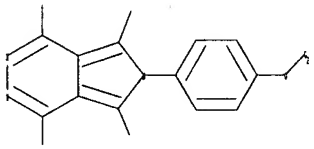

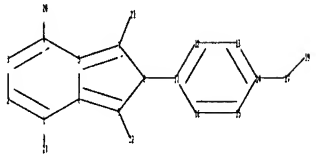

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ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15 16
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ring bonds :
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15-16
exact/norm bonds :
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exact bonds :

1-23 4-20 7-21 9-22
normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16

G1:H,Cy

G2:H,CH3,Et,n-Pr,i-Pr,CF3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS

L10 STRUCTURE UPLOADED

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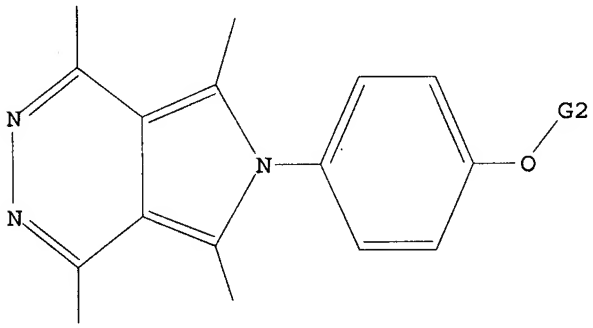
L10 STR



G1 H,Cy
G2 H,Me,Et,n-Pr,i-Pr,CF3

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 138 TO ITERATE

100.0% PROCESSED 138 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

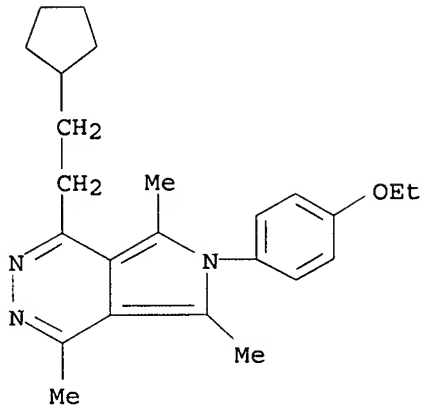
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 2056 TO 3464
PROJECTED ANSWERS: 3 TO 163

L11 3 SEA SSS SAM L10

=> d l11 scan

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 1-(2-cyclopentylethyl)-6-(4-ethoxyphenyl)-
4,5,7-trimethyl-

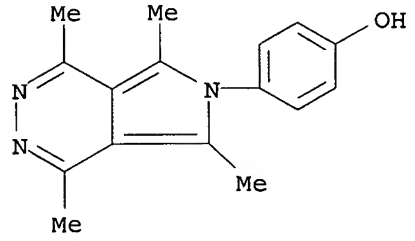
MF C24 H31 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

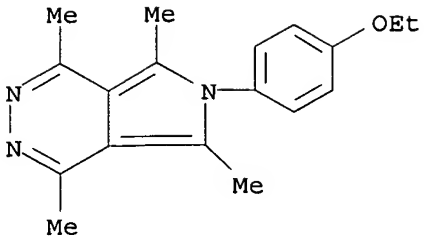
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Phenol, 4-(1,4,5,7-tetramethyl-6H-pyrrolo[3,4-d]pyridazin-6-yl)-
MF C16 H17 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1,4,5,7-tetramethyl-
MF C18 H21 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

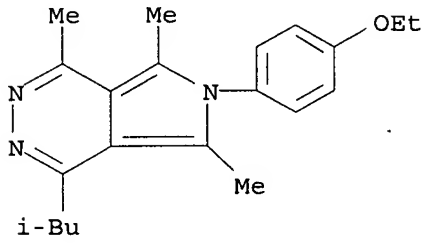
=> s l10 sss full
FULL SEARCH INITIATED 11:35:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2820 TO ITERATE

100.0% PROCESSED 2820 ITERATIONS 54 ANSWERS
SEARCH TIME: 00.00.01

L12 54 SEA SSS FUL L10

=> d l12 scan

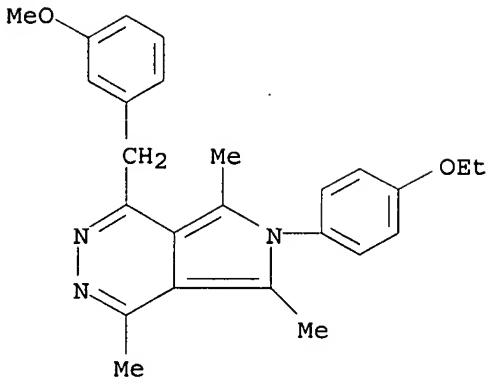
L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1,5,7-trimethyl-4-(2-methylpropyl)-
MF C21 H27 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

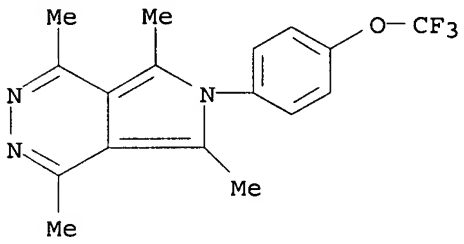
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 6-(4-ethoxyphenyl)-1-[(3-methoxyphenyl)methyl]-4,5,7-trimethyl-
MF C25 H27 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 54 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 6H-Pyrrolo[3,4-d]pyridazine, 1,4,5,7-tetramethyl-6-[4-(trifluoromethoxy)phenyl]-
MF C17 H16 F3 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.90	653.09

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FILE LAST UPDATED: 11 Dec 2007 (20071211/ED)

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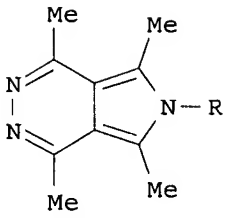
=> s l12
L13 4 L12

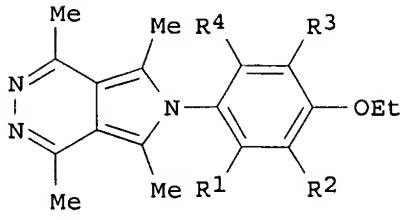
=> d l13 1-4 ti abs bib

L13 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
TI Expedited SAR study of high-affinity ligands to the α2δ subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology
AB The SAR of the lead compound 3, a novel ligand for the α2δ subunit of voltage-gated calcium channels, was rapidly explored. Utilizing a parallel solution-phase Sn2Ar coupling approach, a focused library was obtained. The library was evaluated in vitro and afforded a series of analogs with improved potencies. The SAR trends of the library are also described.
AN 2005:1342000 CAPLUS <<LOGINID::20071212>>
DN 144:100381
TI Expedited SAR study of high-affinity ligands to the α2δ subunit of voltage-gated calcium channels: Generation of a focused library using a solution-phase Sn2Ar coupling methodology
AU Chen, Chixu; Stearns, Brian; Hu, Tao; Anker, Naomi; Santini, Angelina; Arruda, Jeannie M.; Campbell, Brian T.; Datta, Purabi; Aiyar, Jayashree; Munoz, Benitio
CS Department of Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA
SO Bioorganic & Medicinal Chemistry Letters (2006), 16(3), 746-749
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 144:100381
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the α2δ subunit of voltage-gated calcium channels
GI



I



II

AB 2H-pyrrolo[3,4-c]pyridazines I (R = 4-EtOC6H4, 2-EtO-5-pyridinyl, 5-EtO-2-pyridinyl, 5-EtO-2-pyrazinyl, 4-EtO-1-pyridazinyl, 2-EtO-5-pyrimidinyl, etc.) such as II (R1 = H, MeO, Et, H2C:CH, Me, MeS, EtO, F; R2 = H, Me; R3 = H, Me, Cl, HOCH2; R4 = H, Me) are prepared as ligands for the α2δ subunit of voltage-gated calcium channels. Ortho-substituents capable of electron-donation increase the binding of II to the α2δ subunit of voltage-gated calcium channels; electron-withdrawing substituents in the ortho-position of II decrease binding significantly. II (R1 = MeO; R2 = R3 = R4 = H) binds to the α2δ subunit of voltage-gated calcium channels from A710 cells with an IC50 value of 4 nM. Testing of tritiated ligand II (R1 = TCH2TCH; R2 = R3 = R4 = H) in purified human α2δ voltage-gated calcium channel subunits indicates that II displace Gabapentin from the α2δ subunit of voltage-gated calcium channels, and thus act as Gabapentin mimics in vitro. In the preparation of II (R1 = Et; R2 = R3 = R4 = H), a novel metal-free hydrogenation is used using hydrazine as the reductant; the reduction is effective in other systems (no data).

AN 2004:303255 CAPLUS <<LOGINID::20071212>>

DN 141:54277

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives as high-affinity ligands of the α2δ subunit of voltage-gated calcium channels

AU Hu, Tao; Stearns, Brian A.; Campbell, Brian T.; Arruda, Jeannie M.; Chen, Chixu; Aiyar, Jayashree; Bezverkov, Robert E.; Santini, Angelina; Schaffhauser, Herve; Liu, Wensheng; Venkatraman, Shankar; Munoz, Benito

CS MRLSDB2, Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2031-2034 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

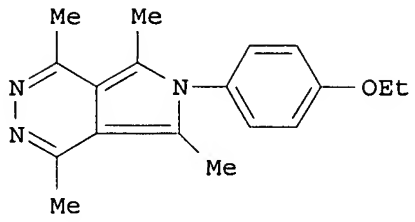
OS CASREACT 141:54277

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the α2δ subunit of voltage gated calcium channels

GI



I

AB A novel class of 6-aryl-6H-pyrrolo[3,4-d]pyridazine ligands for the α2δ subunit of voltage-gated calcium channels has been described. Substitutions in the aryl ring of the mol. were generally not tolerated, and resulted in diminished binding to the α2δ subunit. Modifications to the pyridazine ring revealed numerous permissive substitutions, and detailed SAR studies were carried out in this portion of the mol. Replacement of the pyridazine ring Me group with an aminomethyl functionality provided greatly improved potency over the initial lead. The initial lead compound (I) displayed good rat pharmacokinetic properties, and was shown to be efficacious in the Chung model for neuropathic pain in rats.

AN 2004:153601 CAPLUS <<LOGINID::20071212>>

DN 140:357282

TI Synthesis and biological evaluation of 6-aryl-6H-pyrrolo[3,4-d]pyridazine derivatives: high-affinity ligands to the α2δ subunit of voltage gated calcium channels

AU Stearns, Brian A.; Anker, Naomi; Arruda, Jeannie M.; Campbell, Brian T.; Chen, Chixu; Cramer, Merryl; Hu, Tao; Jiang, Xiaohui; Park, Kenneth; Ren, Kun Kun; Sablad, Marciano; Santini, Angelina; Schaffhauser, Herve; Urban, Mark O.; Munoz, Benito

CS Department of Medicinal Chemistry, Merck Research Laboratories, San Diego, CA, 92121, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(5), 1295-1298
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

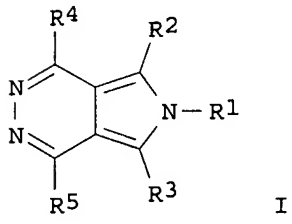
OS CASREACT 140:357282

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 4 CAPLUS

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds

GI



I

AB The title compds. [I; R1 = (un)substituted alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl; R2-R5 = a bond, (un)substituted alkyl, alkyl(hetero)aryl, alkyl(hetero)cycloalkyl, (hetero)aryl, (hetero)cycloalkyl] were prepared as as ligands of voltage

gated calcium channels (VGCC), useful in the treatment of neuropathic pain, and psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson s disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, drug addiction, drug abuse, drug withdrawal and other. E.g., a multi-step synthesis of I [R1 = 4-EtOC6H4; R2-R4 = Me; R5 = 4-MeOC6H4] which produced a 65% effect after i.p. dosing at 30 mg/kg in spinal nerve ligation model of neuropathic pain in rats, was given. The pharmaceutical composition comprising the compound I is claimed.

AN 2004:60243 CAPLUS <<LOGINID::20071212>>

DN 140:111422

TI Treatment of neuropathic pain with 6H-pyrrolo[3,4-d]pyridazine compounds

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	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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